Multiscale Fuel Performance Modeling

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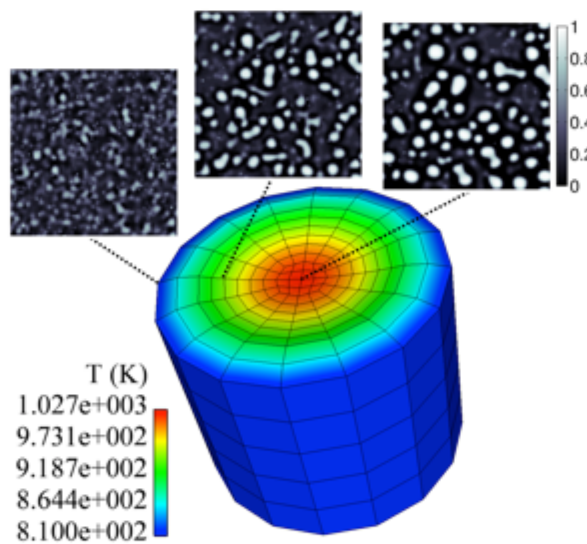


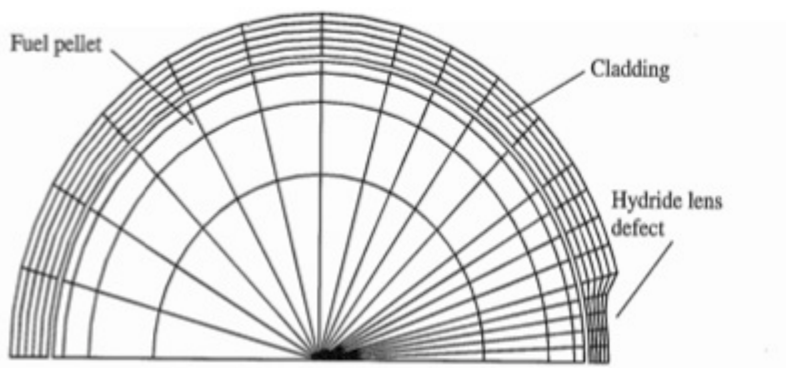
LWR Fuel Behavior Modeling – U.S. State of the Art

- Fuel performance codes are used today for determination of operational margins by calculating property evolution.
- However, current industry standard codes (e.g. FRAPCON and FALCON) have significant limitations in three main areas:

Numerical Capabilities
- Serial
- Inefficient Solvers
- Loosely Coupled
- High Software Complexity

Geometry representation
- 1.5 or 2-D
- Smeared Pellets
- Restricted to LWR Fuel

Materials models
- Empirical
- Models only valid in limited conditions
- Limited applicability in accident scenarios

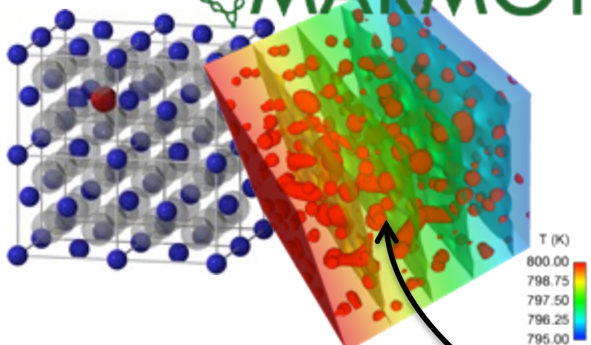


FALCON model to investigate clad failure due to defect

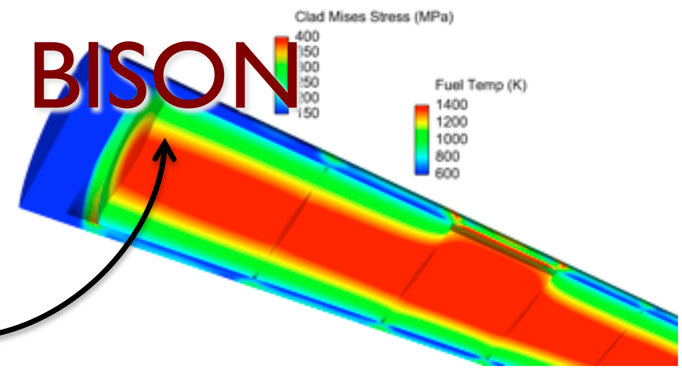
MOOSE-BISON-MARMOT

- The MOOSE-BISON-MARMOT codes provide an advanced, multiscale fuel performance capability

MARMOT



BISON



Atomistic/Mesoscale Material Model Development

- Predicts microstructure evolution in fuel
- Used with atomistic methods to develop multiscale materials models

Advanced 3D Fuel Performance Code

- Models LWR, TRISO and metal fuels in 2D and 3D
- Steady and transient reactor operations

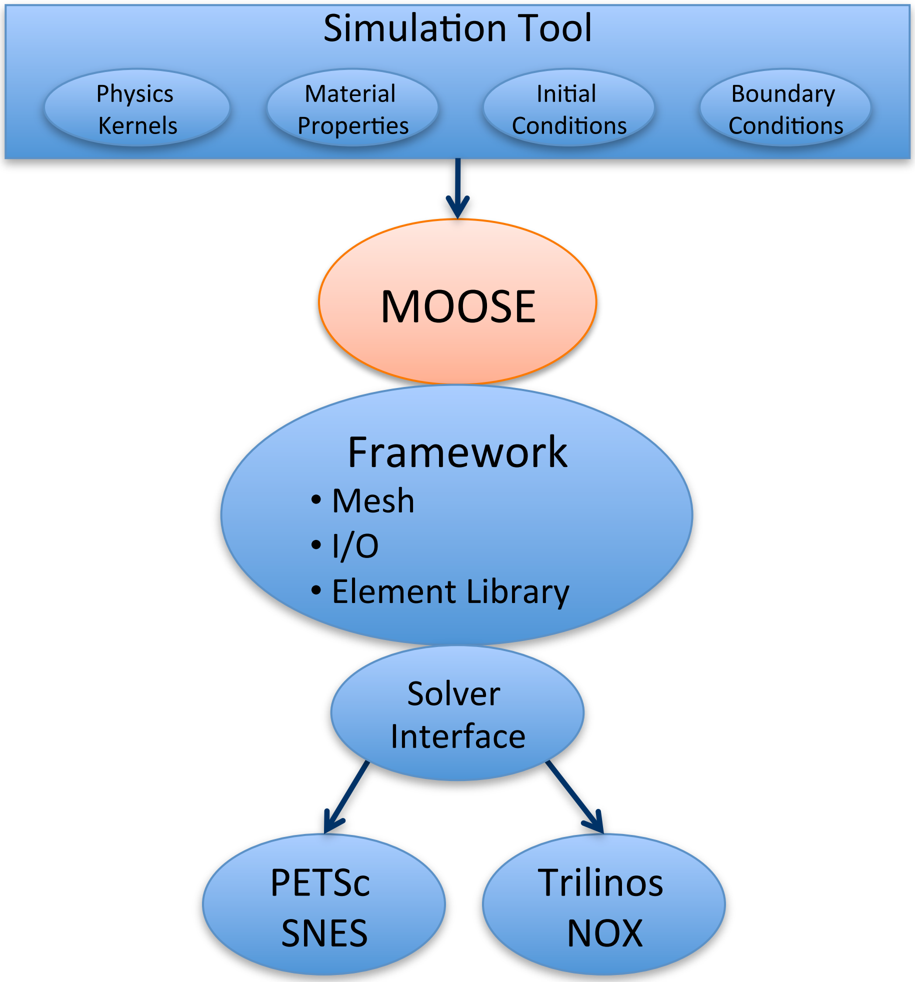
MOOSE

Multiphysics Object-Oriented Simulation Environment

- Simulation framework allowing rapid development of FEM-based applications

MOOSE: Multiphysics Object-Oriented Simulation Environment

- MOOSE is an object-oriented FEM framework allowing rapid development of new simulation tools.
- Solves systems of coupled partial differential equations
- Leverages multiple DOE and university developed scientific computational tools
- Allows scientists and engineers to efficiently develop state of the art simulation capabilities.
  - **Maximize Science/$**
- Has been licensed by multiple national labs, universities and private industry

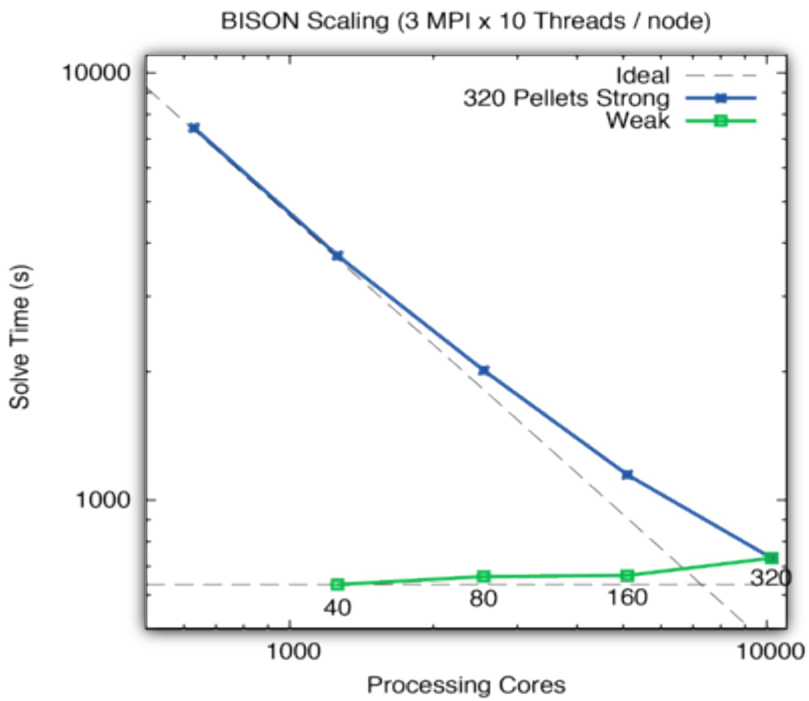


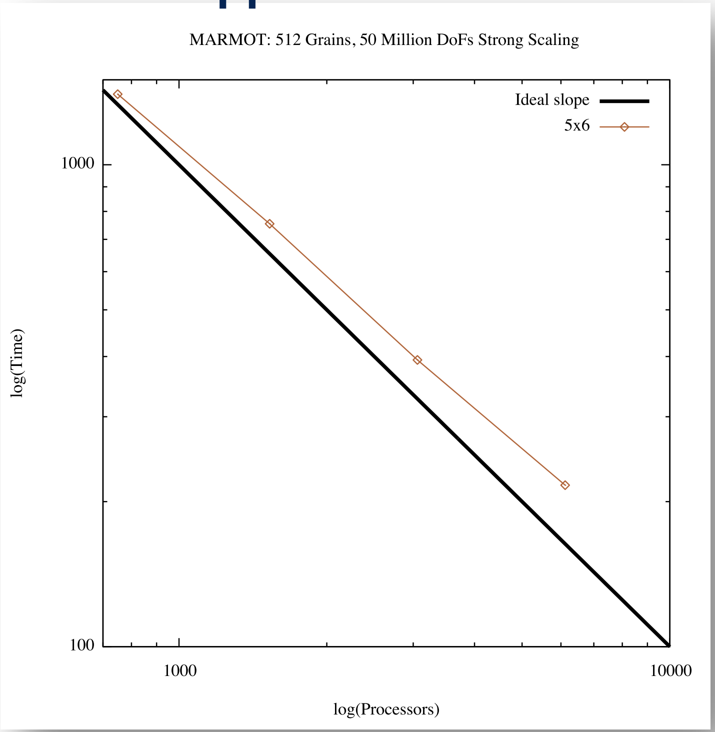
Los Alamos National Laboratory EST.1943 · Argonne National Laboratory · ANATECH · Oak Ridge National Laboratory · Pacific Northwest National Laboratory · Bettis Laboratory · MIT Massachusetts Institute of Technology · Michigan · The University of Wisconsin Madison

MOOSE Capabilities

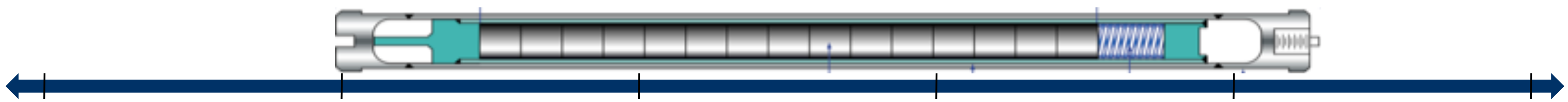
- Same user code works in 1D, 2D and 3D
- Fully coupled, fully implicit
- Mesh and time step adaptivity
- Massively parallel without requiring user to write parallel code

Parallel scalability plots from two MOOSE applications





Microstructure Evolution in LWR Fuel



Insertion in reactor

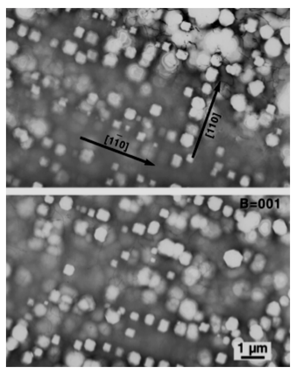
Removal from reactor

Early life
- Thermal expansion
- Fracture
- Point defect and fission gas generation
- Fuel Densification

Mid Life
- Point defect diffusion
- Point defect clustering
- Fission gas segregation to GB and voids
- Bubble nucleation

Late life
- Fission product swelling
- Bubble percolation and fission gas release
- Cladding creep
- Fuel creep

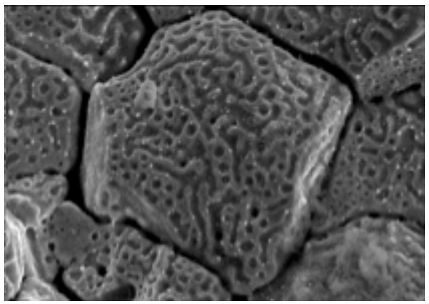
Fuel failure
- Pellet/cladding interaction
- Cladding corrosion
- Cladding fracture

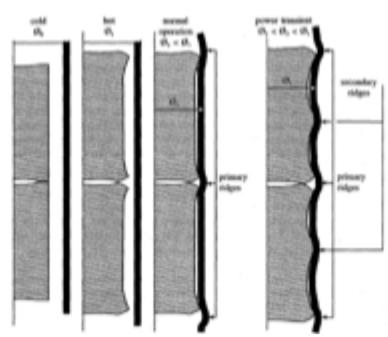


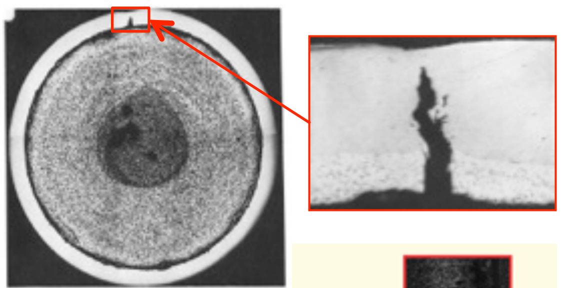
Zinkle and Singh 2000

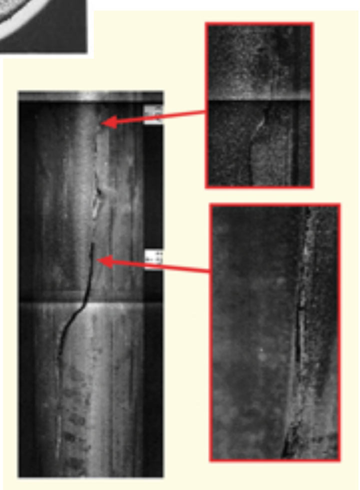
Olander, p. 323 (1978)

Brohan 2000



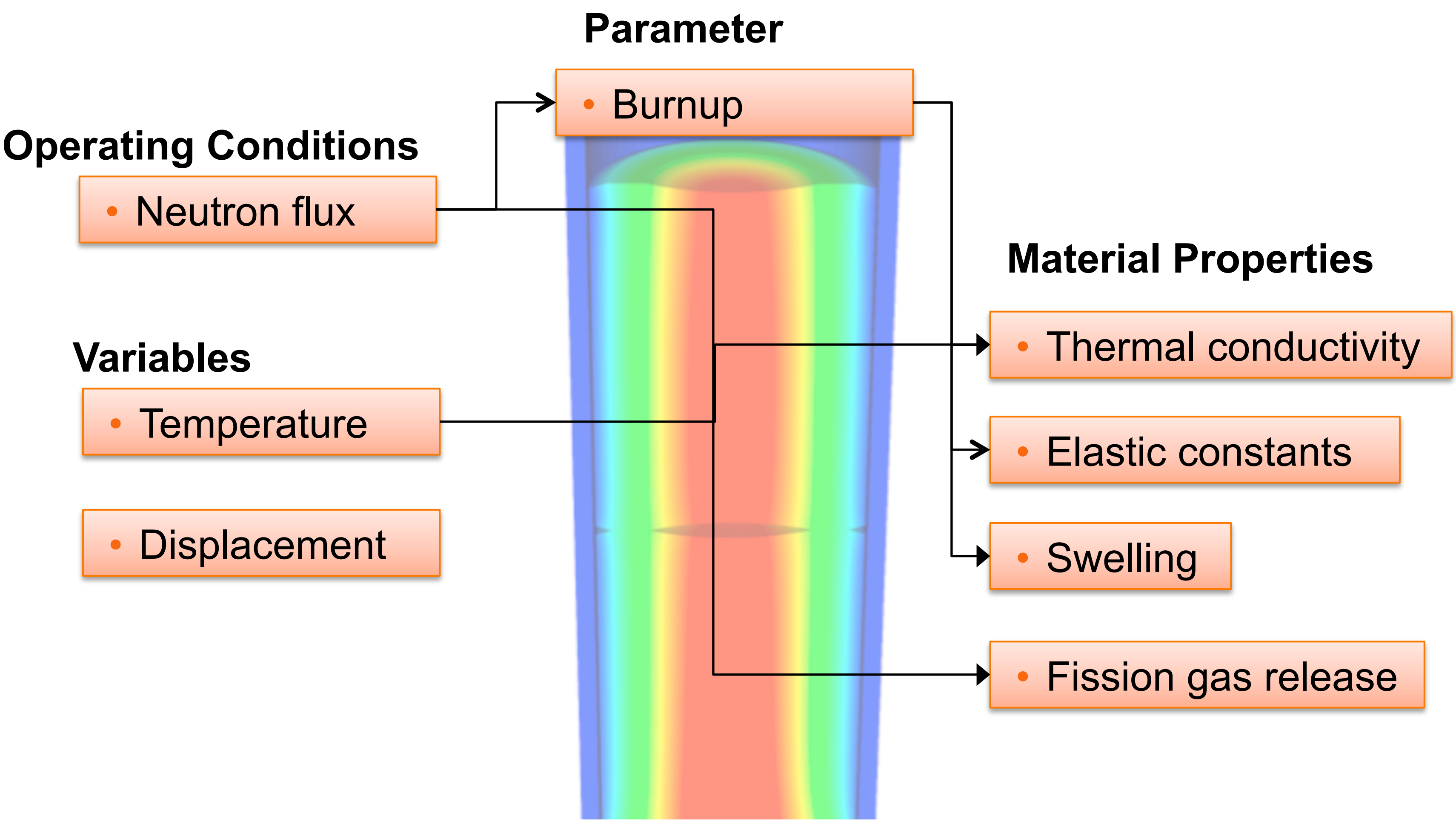






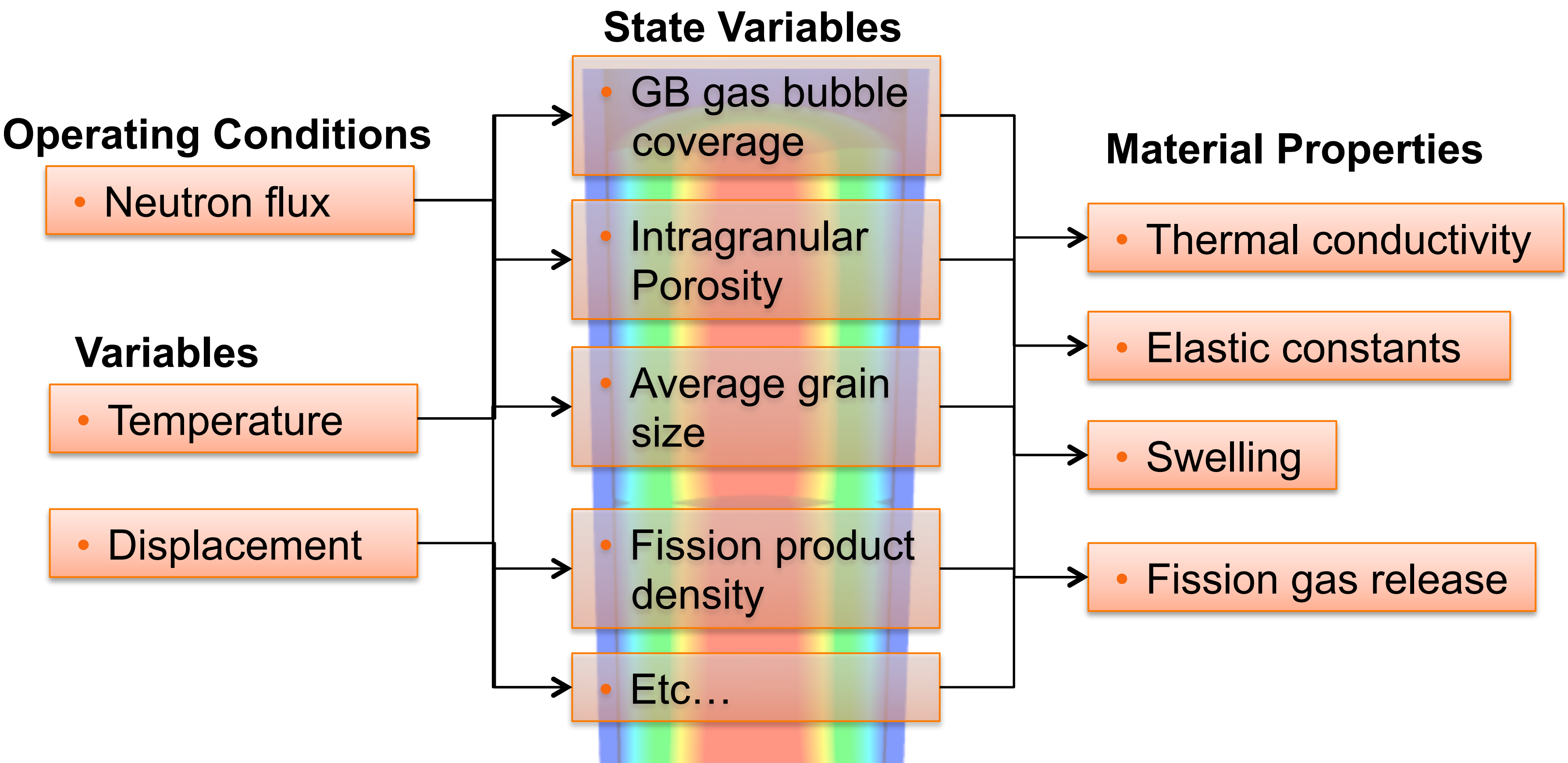
LWR Fuel Performance Modeling – U.S. State of the Art

- Current materials models are empirical fits of LWR data, and are correlated to burnup and temperature



Proposed State Variable Model

- Microstructure of the material is represented by state variables

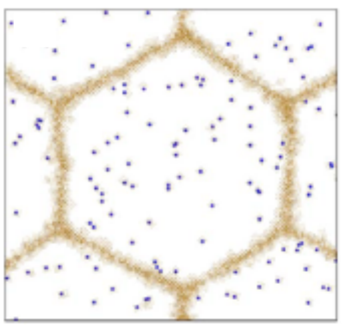


- Expression are needed to define state variable evolution and their influence on material properties

Multiscale Modeling Approach

- Though experiments may provide some information about the state variables, modeling and simulation provides another valuable tool
- ***Research goal***: *To develop state variable (SV) evolution expressions to define microstructure and its influence on material properties*

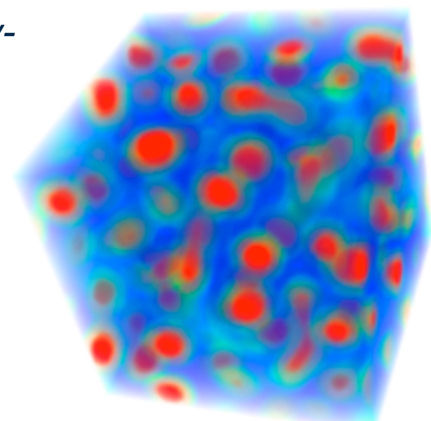
Atomistic simulation



- Identify important mechanisms
- Determine material parameter values

Atomistically-informed parameters

Mesoscale models

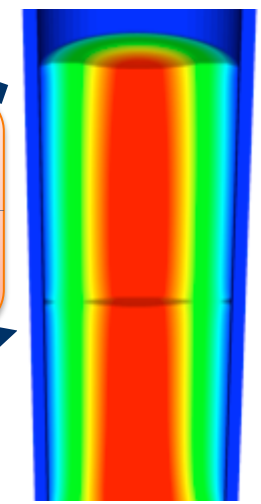


- Predict and define microstructure and state variable evolution
- Determine effect of evolution on material properties

Degrees of freedom, operating conditions

Mesoscale-informed SV models

Fuel performance models



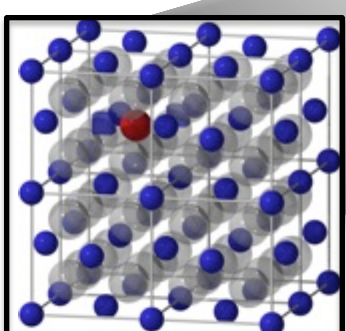
- Predict fuel performance and failure

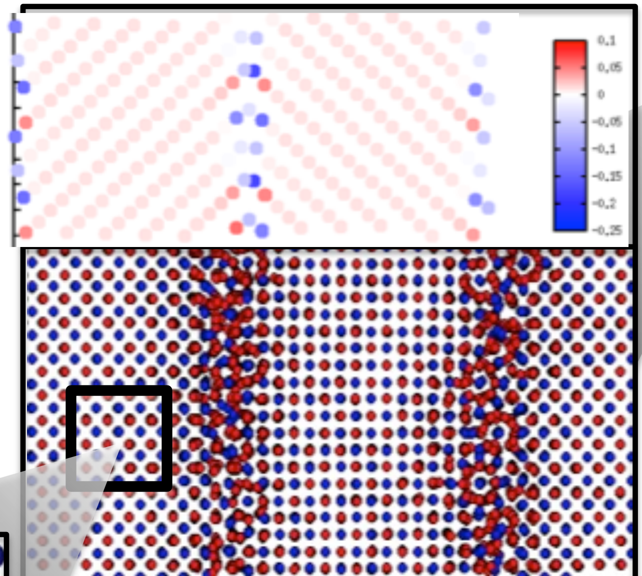
Multiscale Modeling Approach

Modeling Approach: *To develop improved, science-based materials models for fuel performance using hierarchical multiscale modeling*

1st Principles Simulations

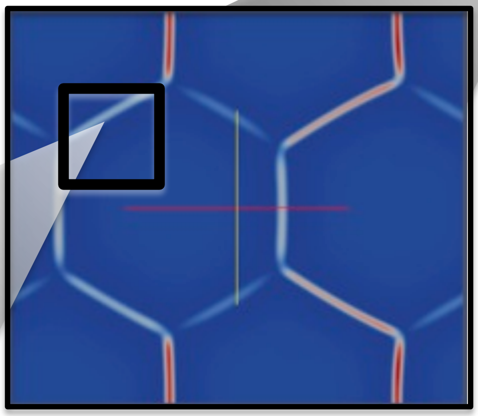
- Identify important bulk mechanisms
- Determine bulk material parameter values





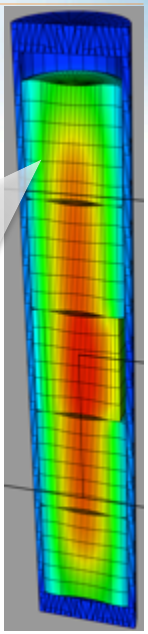
Molecular Dynamics Simulations

- Investigate role of idealized grain boundaries
- Determine grain boundary properties



MARMOT

- Predict and define microstructure state variable evolution
- Determine effect of evolution on material properties



BISON-Peregrine

- Predict fuel performance during operation and accident conditions

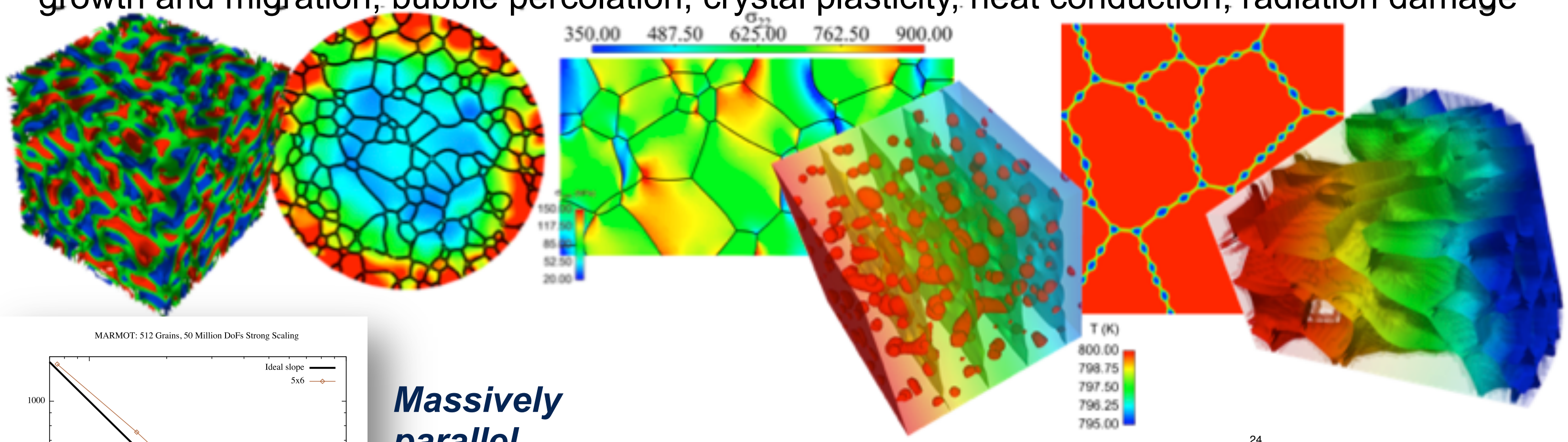
MARMOT *Multiphysics Phase Field Model*

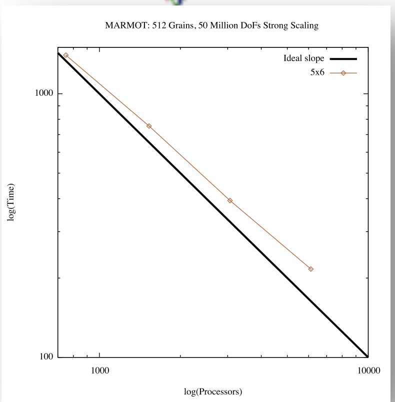
- Determine microstructure and chemical evolution due to applied load, temperature gradients and radiation damage.

Technique: Phase field coupled with solid mechanics and heat conduction

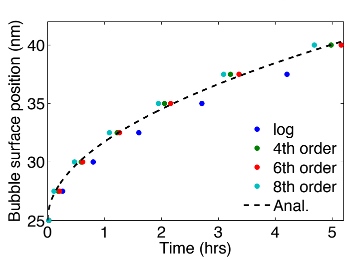
Solution method: Implicit finite element using MOOSE framework

Physical phenomena: Grain growth, GB segregation, GB/pore interaction, pore nucleation, growth and migration, bubble percolation, crystal plasticity, heat conduction, radiation damage

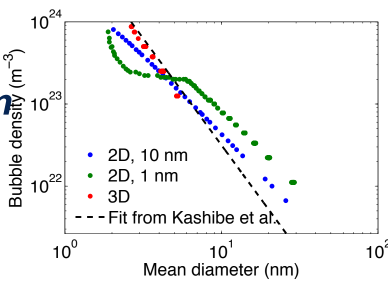




Massively parallel, can be run on 1 cpu or >1000 cpus



Verification and validation is carried out for each model



MARMOT Progress

- Two journal articles specifically on MARMOT have been published, with two under revision and four in progress

ELSEVIER
Computational Materials Science
Volume 51, Issue 1, January 2012, Pages 20–29

An object-oriented finite element framework for multiphysics phase field simulations

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http://dx.doi.org/10.1016/j.commatsci.2011.07.028, How to Cite or Link Using DOI

ELSEVIER
Computational Materials Science
Volume 56, April 2012, Pages 161–165

Phase-field modeling of temperature gradient driven pore migration coupling with thermal conduction

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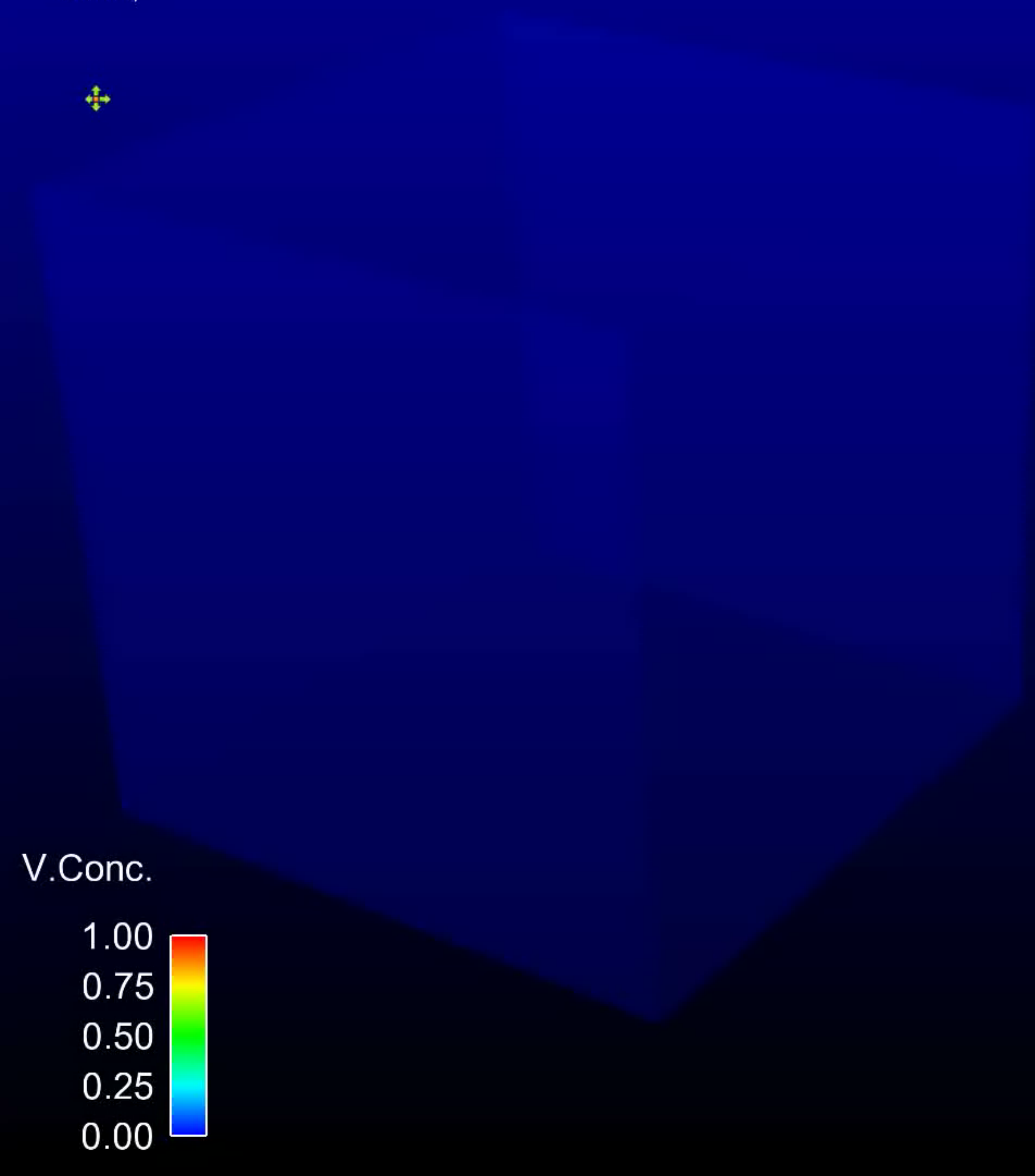
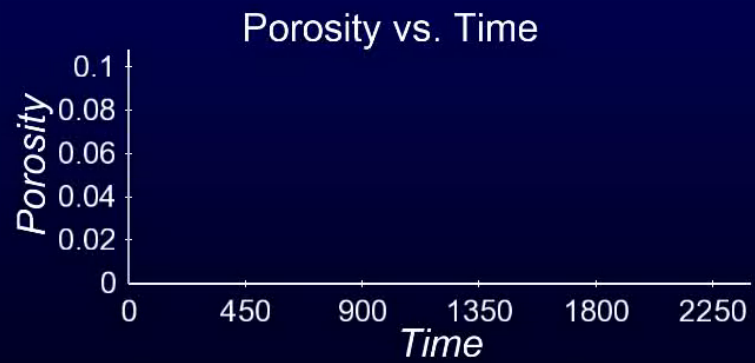
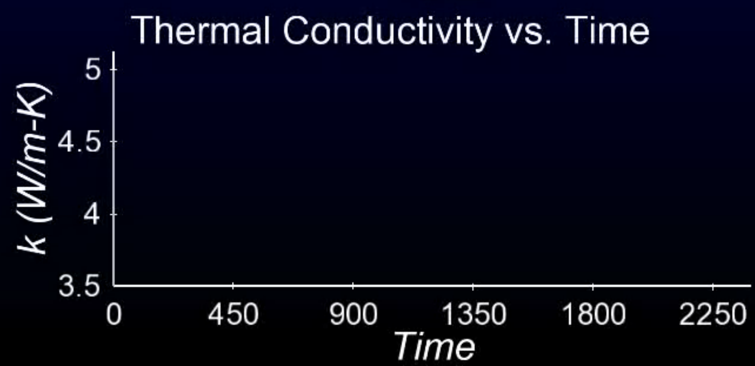
Received 6 December 2011. Accepted 7 January 2012. Available online 7 February 2012.
http://dx.doi.org/10.1016/j.commatsci.2012.01.002, How to Cite or Link Using DOI

- MARMOT is in use by researchers at various laboratories and universities

The Effect of Void Formation on Thermal Conductivity

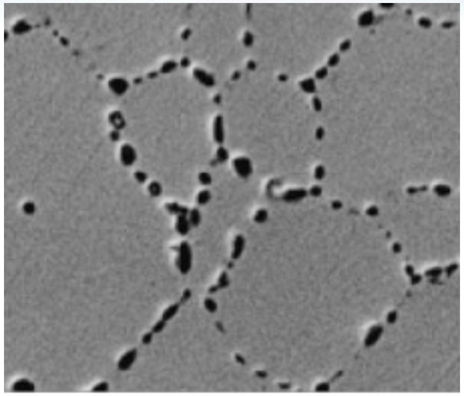




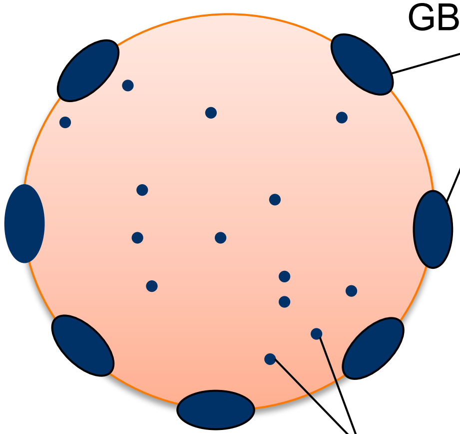


Preliminary State Variable Model

- We have initially developed a simple state variable model that only considers fission gas effects
- We consider two state variables
  - Intragranular gas bubble density
  - Grain boundary (GB) coverage
- The 2-stage Forsberg-Massih fission gas release model is used to evolve the state variables



Forsberg & Massih, J. Nucl. Mater. 135 (1985) 140-148

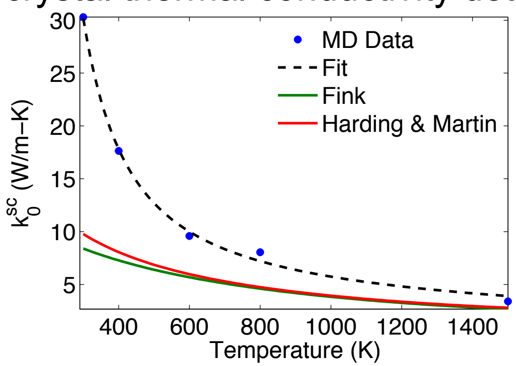


Effect of Fission gas on Thermal Conductivity

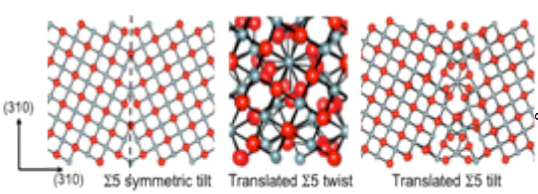
- Goal: Determine how fission gas within the fuel effects the bulk thermal conductivity

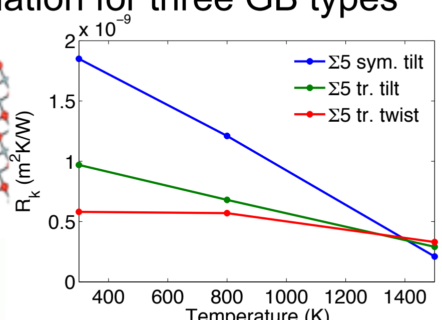
Atomistic

- Single crystal thermal conductivity determined with MD



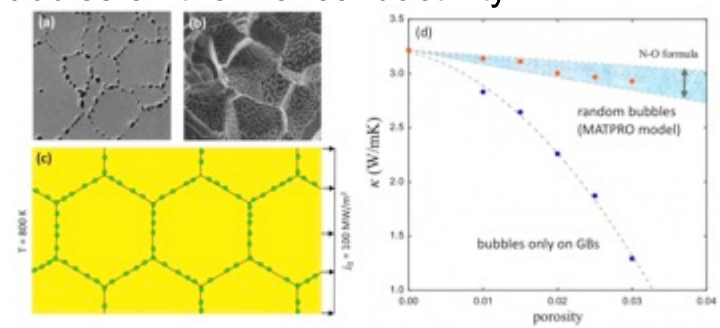
- The UO_2 grain boundary thermal resistance is calculated using MD simulation for three GB types



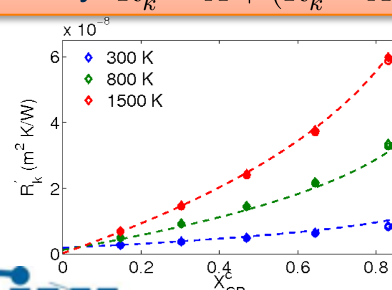


Mesoscale

- Heat conduction simulations investigate the effect of bubbles on thermal conductivity

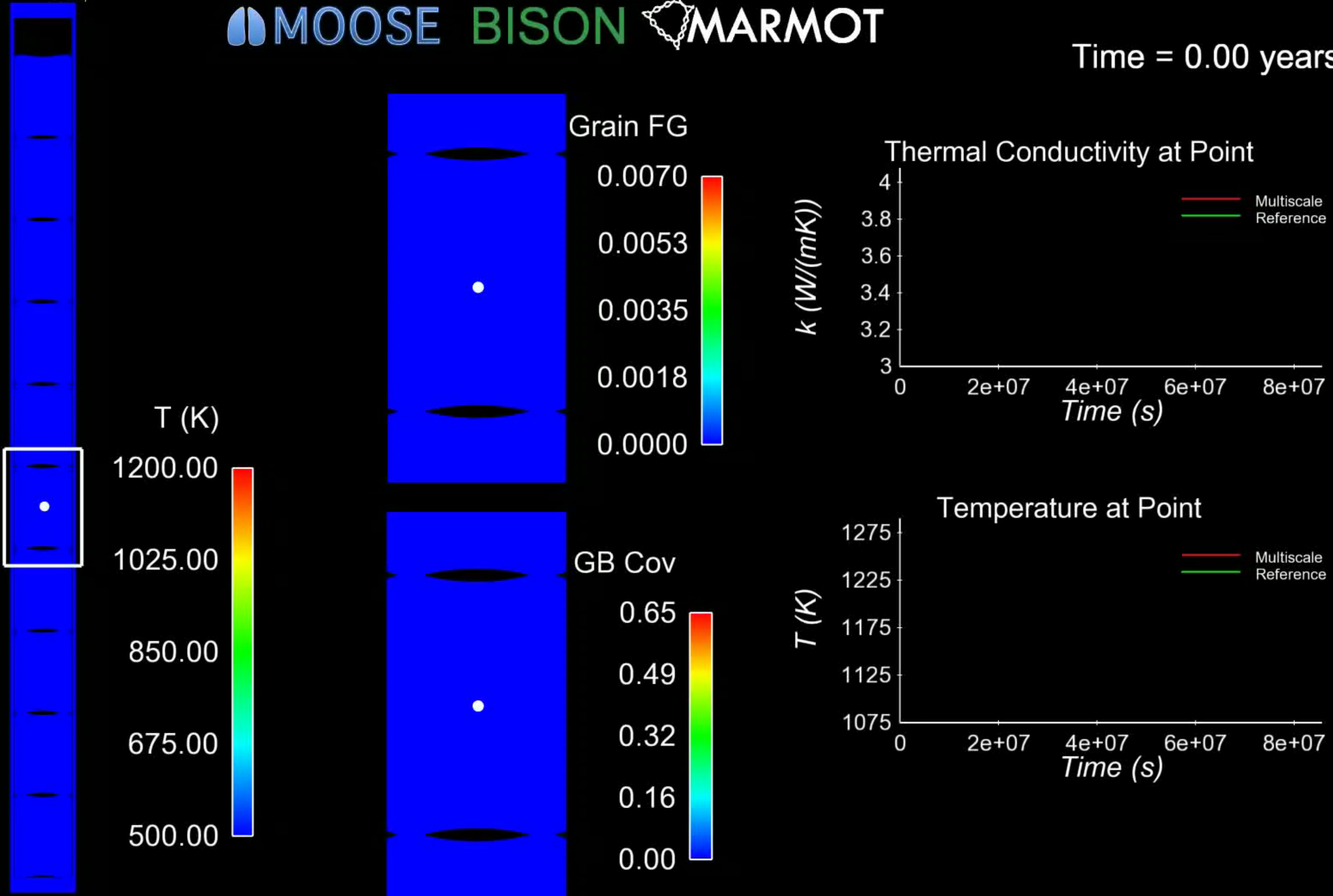


Bubble configuration has a large impact on thermal conductivity: $R_k' = A + (R_k^0 - A)(1 - X_{GB}^C)$



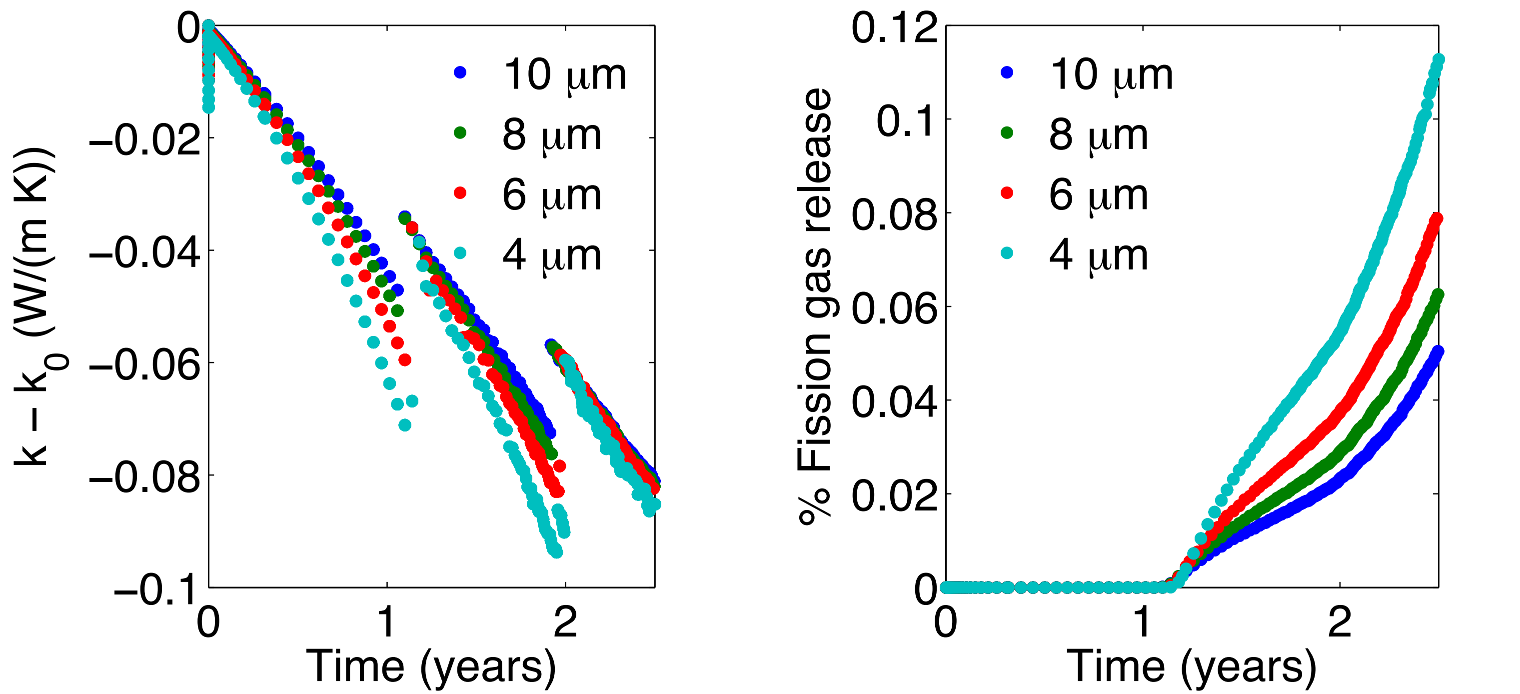
LWR Fuel Rodlet with Multiscale Thermal Conductivity Model

MOOSE BISON MARMOT



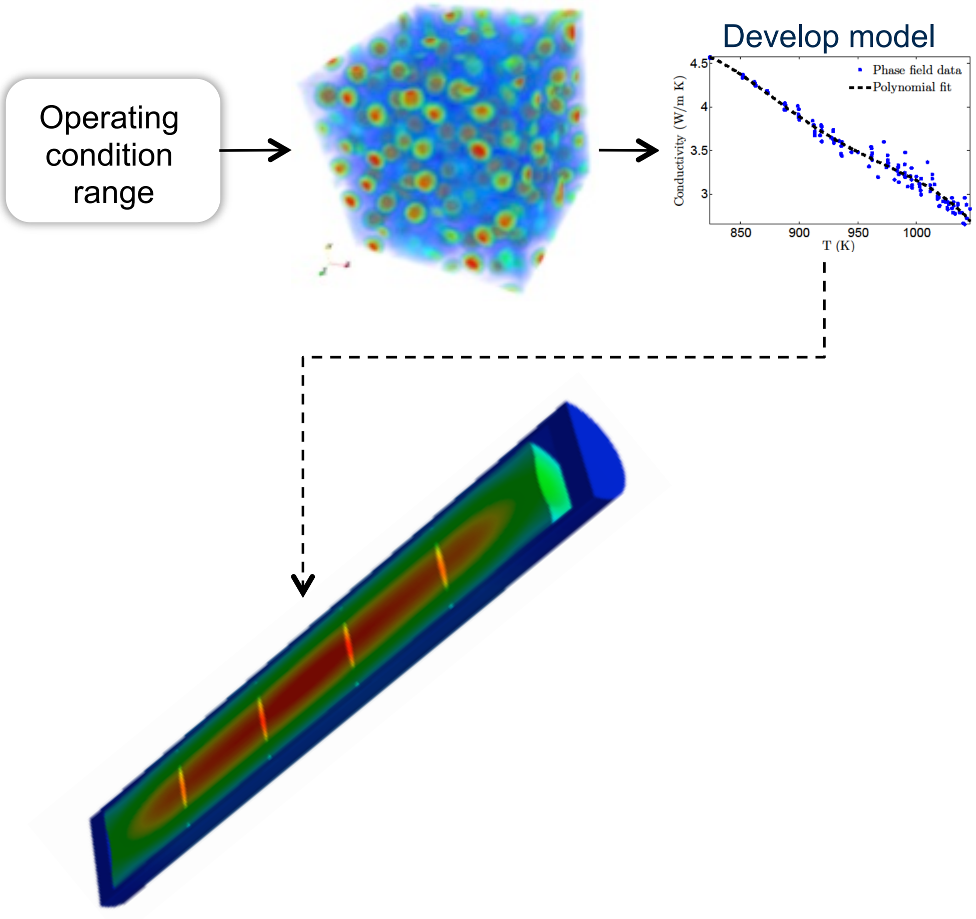
Investigation of Grain Size Effects on Thermal Conductivity

- State variable models capture the effect of microstructure on various aspects of the fuel behavior
  - Here, changing the grain size decreases the fuel thermal conductivity and increases the fission gas release.

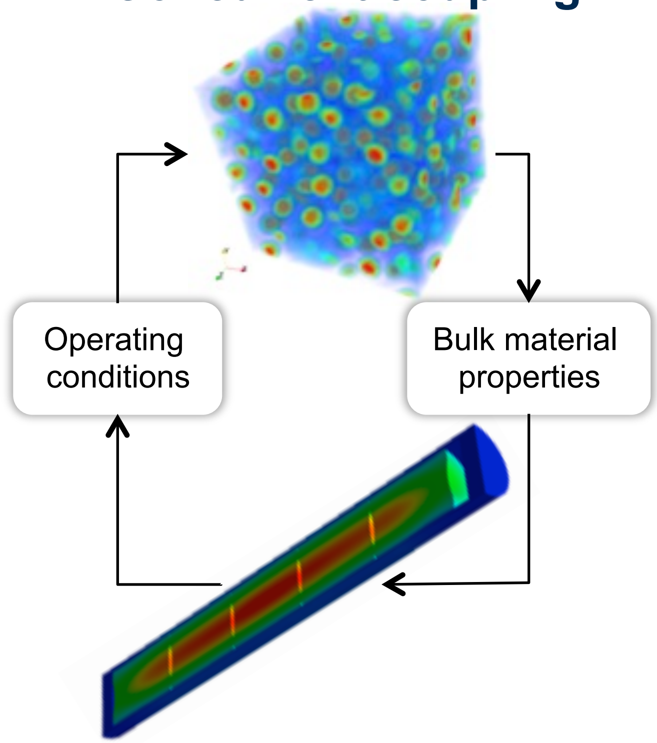


Multiscale Coupling Methods

- Physics-based materials model are developed from the mesoscale simulation results

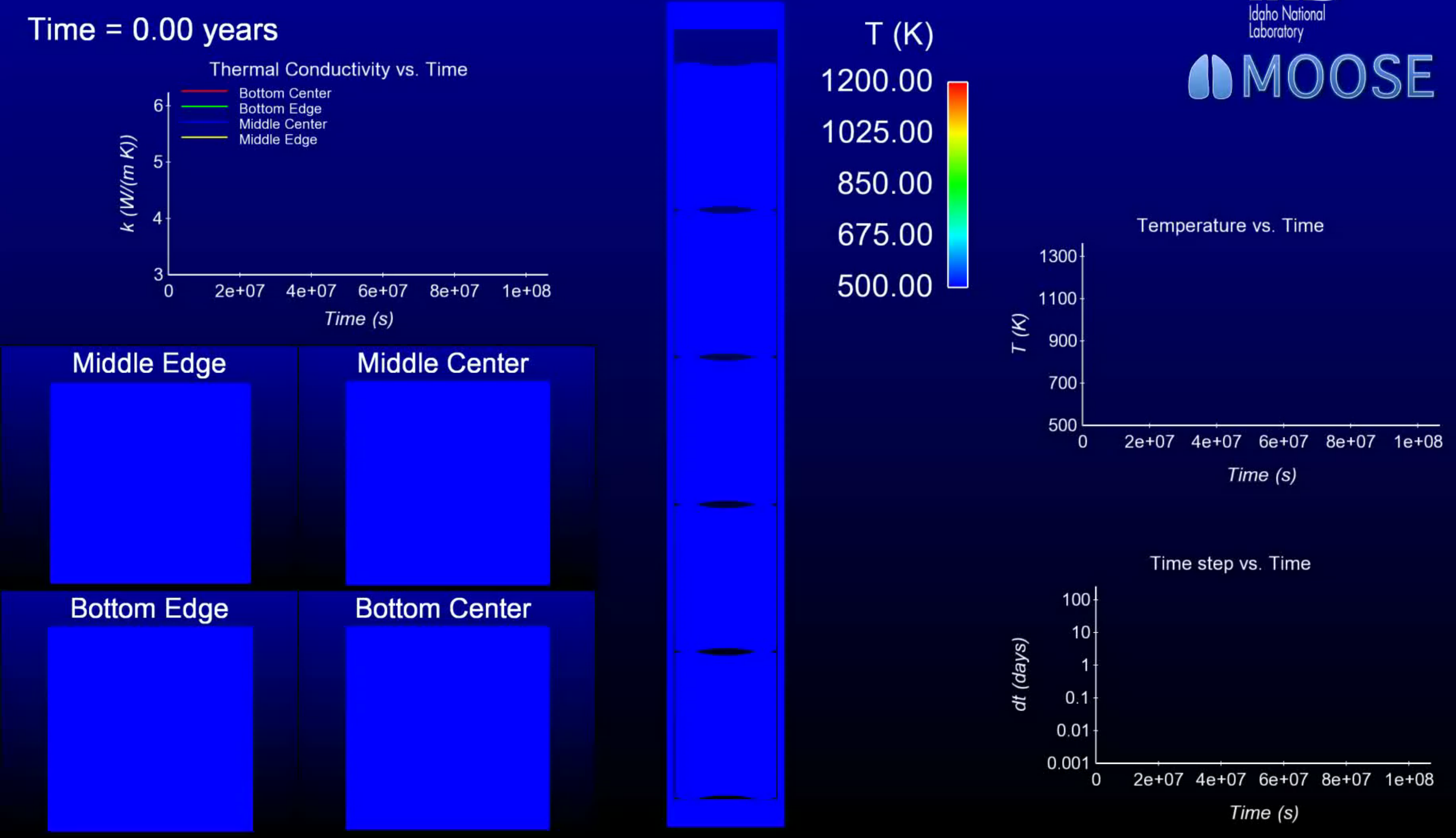


Concurrent coupling



- Another tool for developing materials models
- Captures interaction between the scales
- Can locate important coupled behaviors
- More computationally expensive

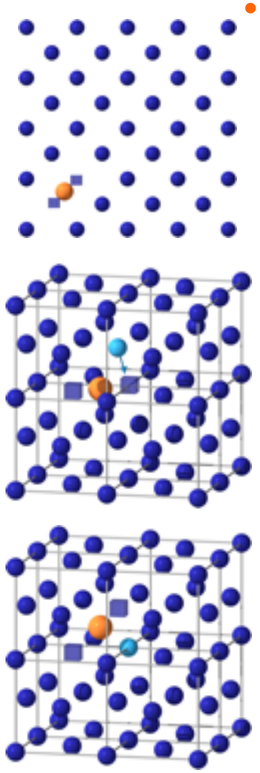
Multiscale UO_2 Fuel Rodlet Simulation



Post-Irradiation Annealing Model

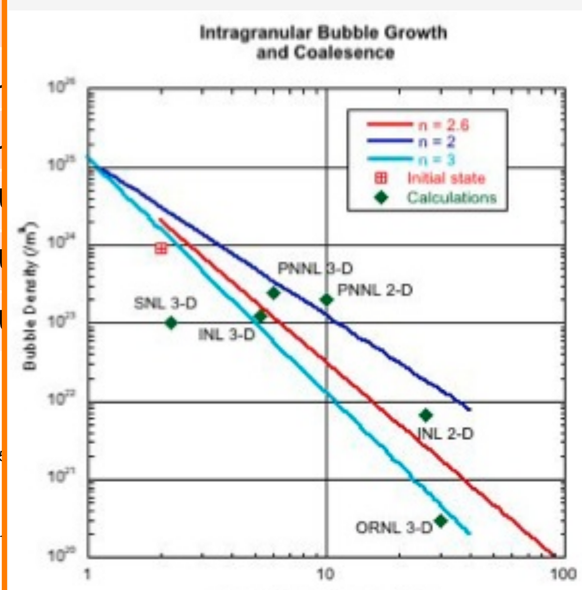
Goal: To validate UO_2 bubble growth models against experimental data

Atomistic



- 1st principles calculations of bulk Xe diffusion in UO_2

	Calc.	Exp[1]
E_a^U(U		
E_a^U (U		
E_a^U (U		
E_a^{Xe} (		
E_a^{Xe} (		
E_a^{Xe} (		

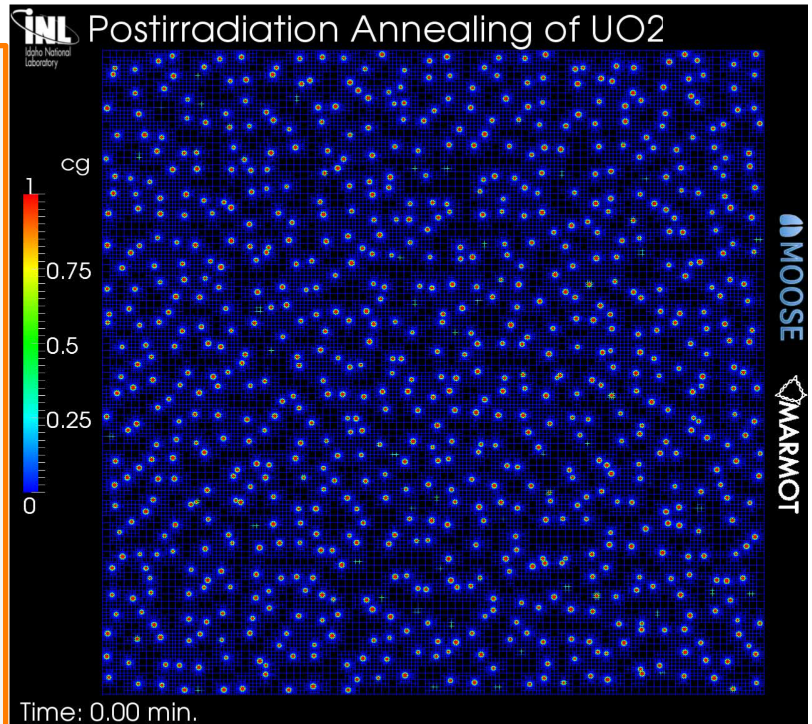


Our results compared well to the data due to our reliance on atomistic data

[1] *Hj. Matzke, in Diffusion Processes in Nuclear Materials, ed. R. P. Agarwala, North-Holland, Amsterdam, 1992.*

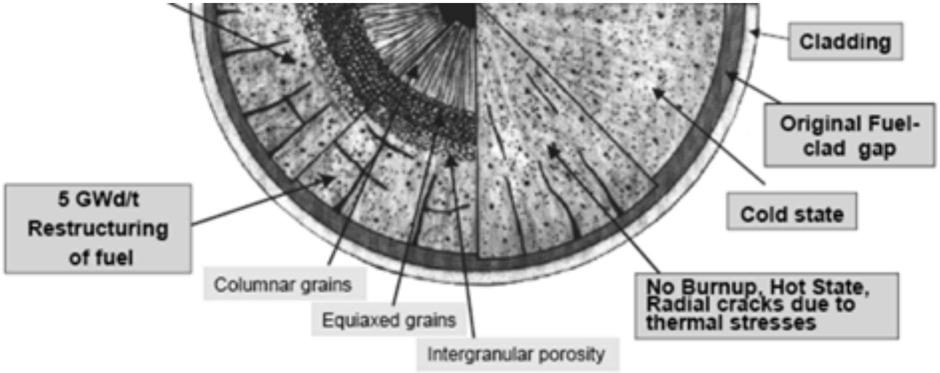
Mesoscale

- Simulation predicts bubble growth during post-irradiation annealing

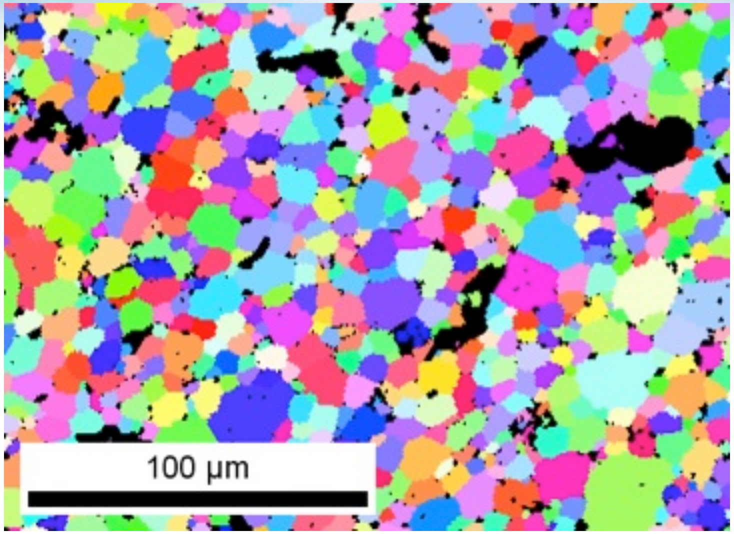


Fuel Restructuring

- Ultimate goal: Predict grain size, pore size and pore density as a function of temperature, stress and neutron flux.



- To understand the fuel restructuring, we are sequentially investigating the contributing driving forces and evolution behaviors



Initial porosity and grains redistribute due to temperature and stress gradients in the fuel (EBSD scan of sintered dUO_2 courtesy of Pedro Peralta from ASU)

Evolution Behaviors:

- GB migration
- Pore migration
- GB and pore interaction

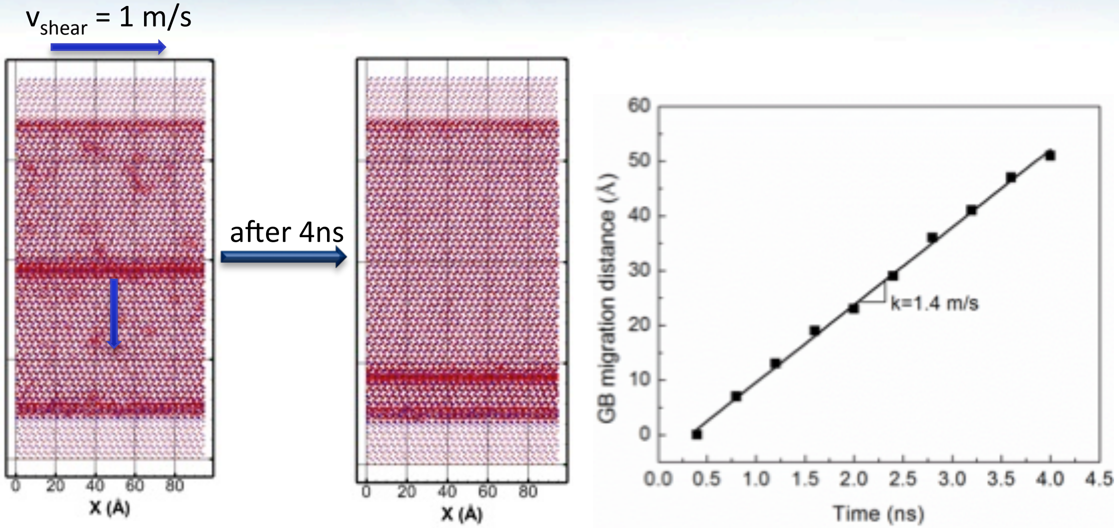
Driving forces:

- Temperature gradient
- Stress gradient
- Combination
- Radiation (future work)

GB Migration

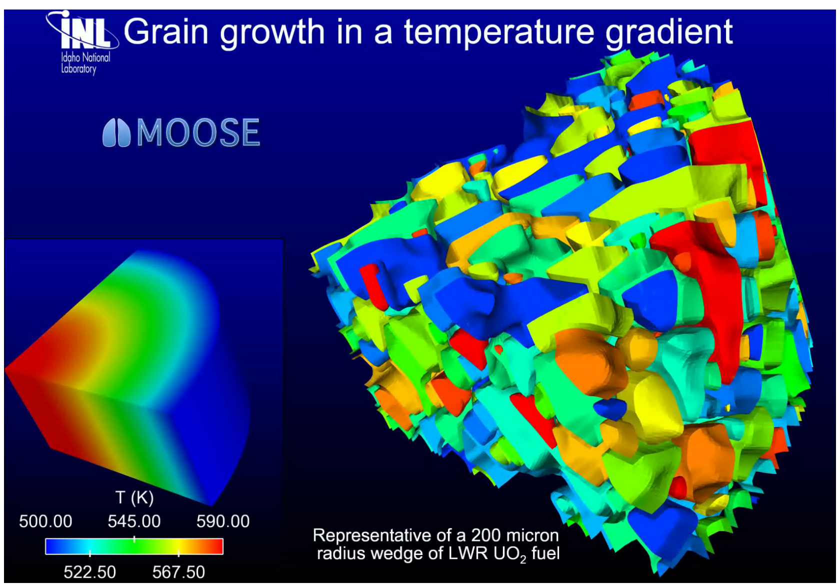
Atomistic

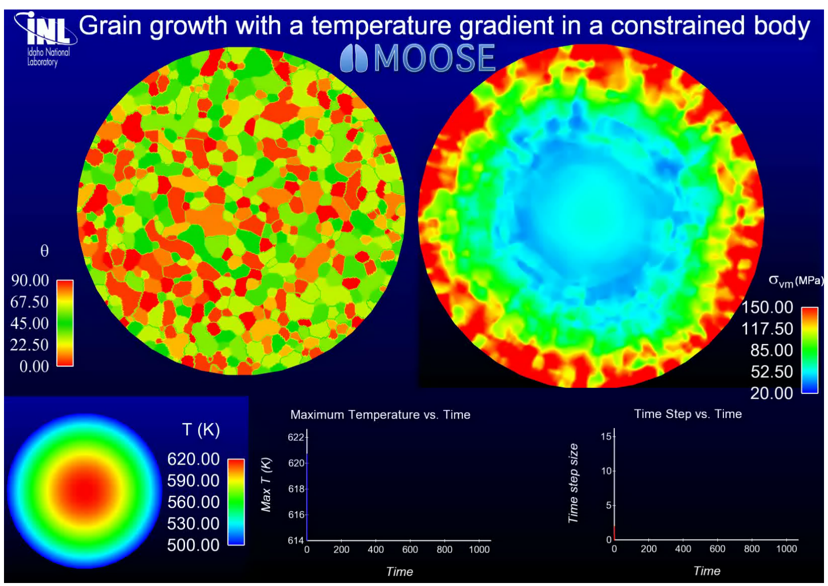
- MD simulations determine the GB mobility due to various driving force



Mesoscale

- MARMOT simulations investigate the effect of the driving forces

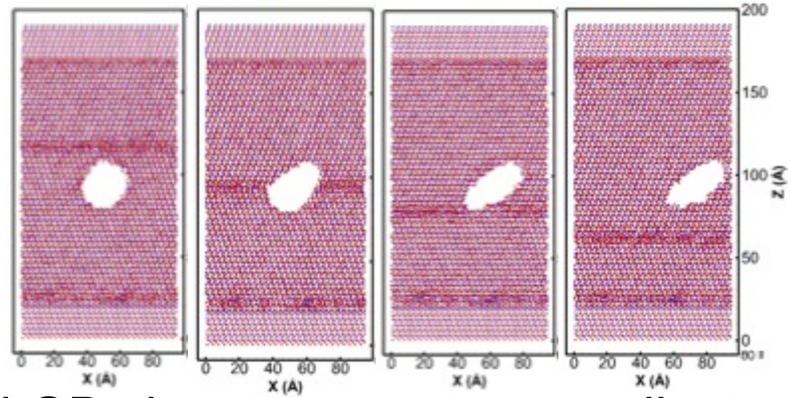




Void/Grain Boundary Interaction

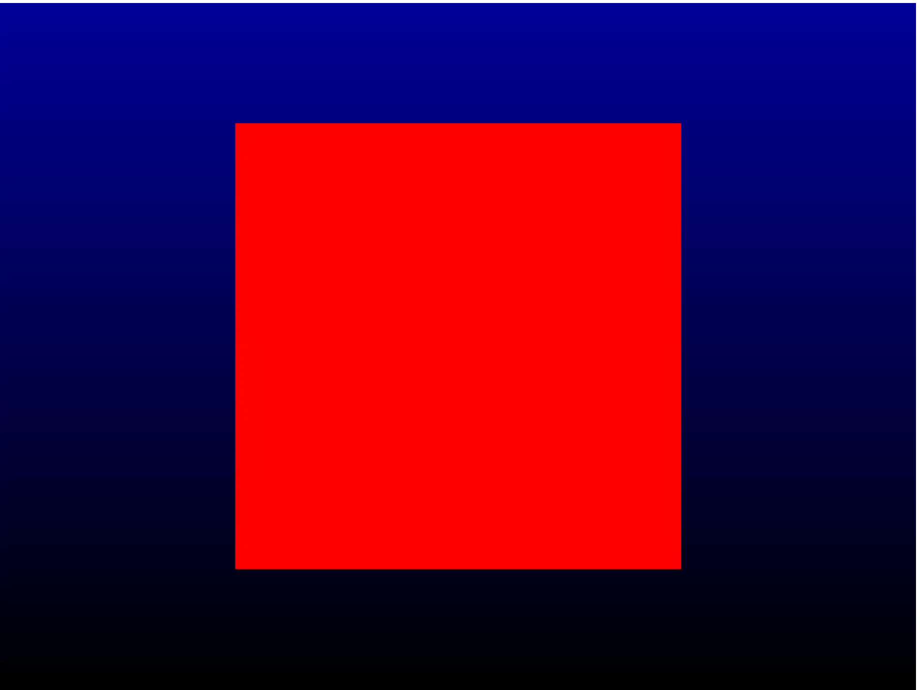
Atomistic

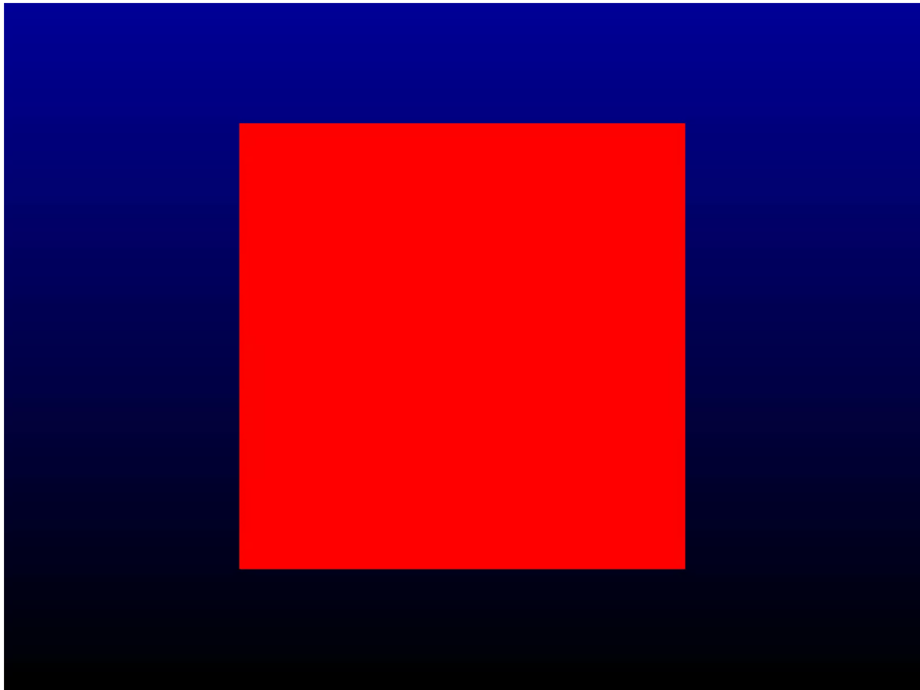
- Mechanistic investigation of void/GB interaction in UO_2



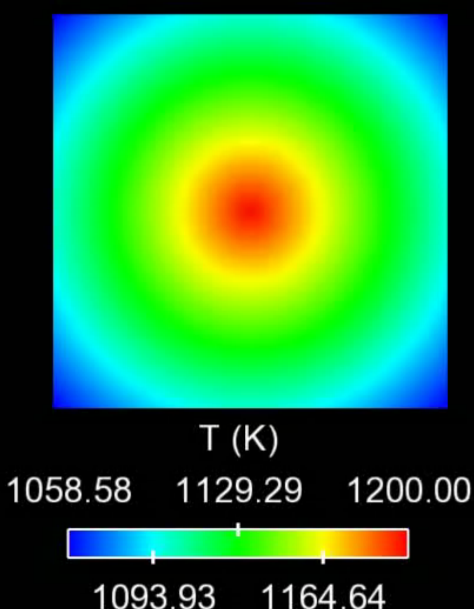
Mesoscale

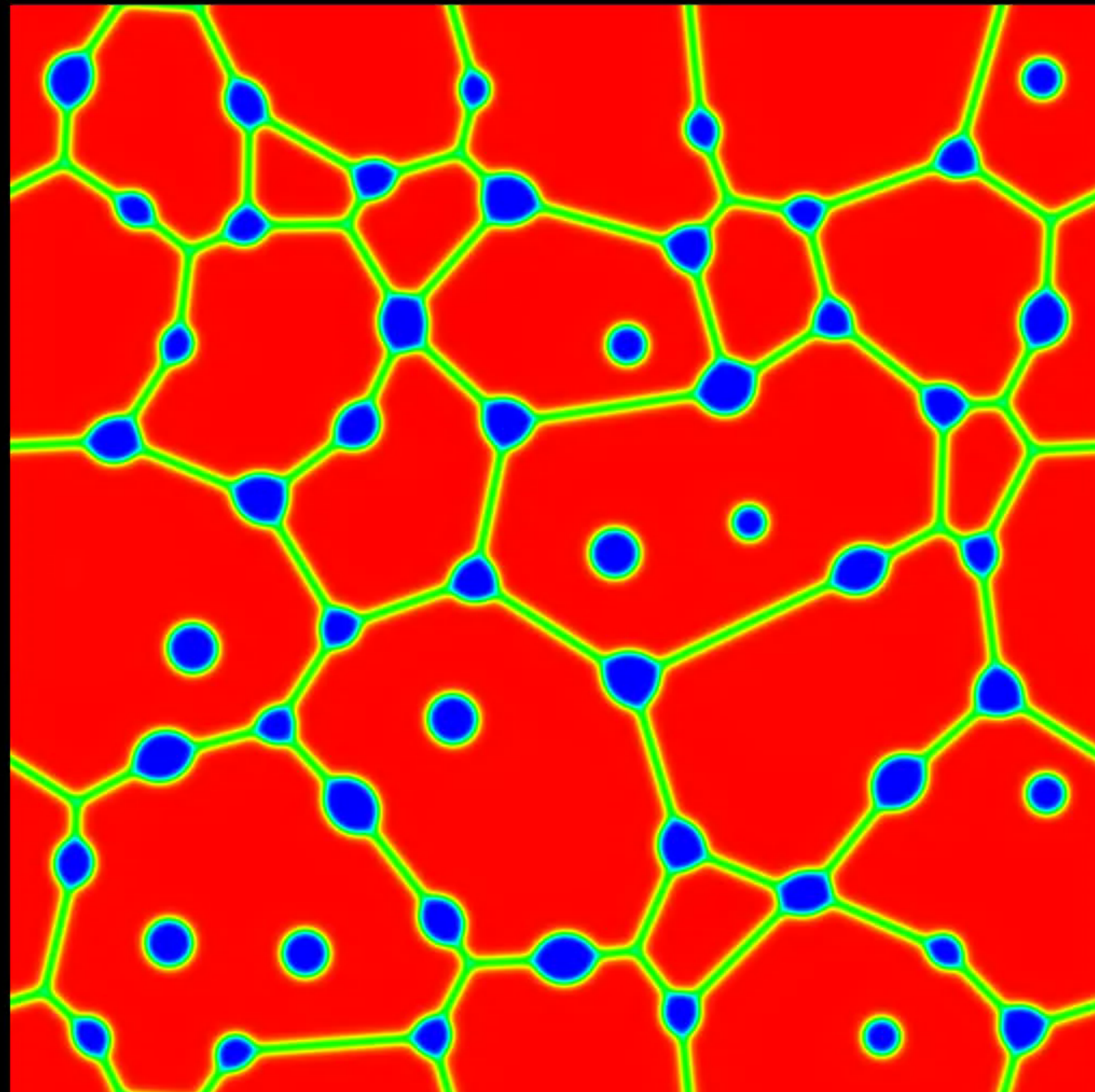
- The interaction between voids and GBs in a temperature gradient





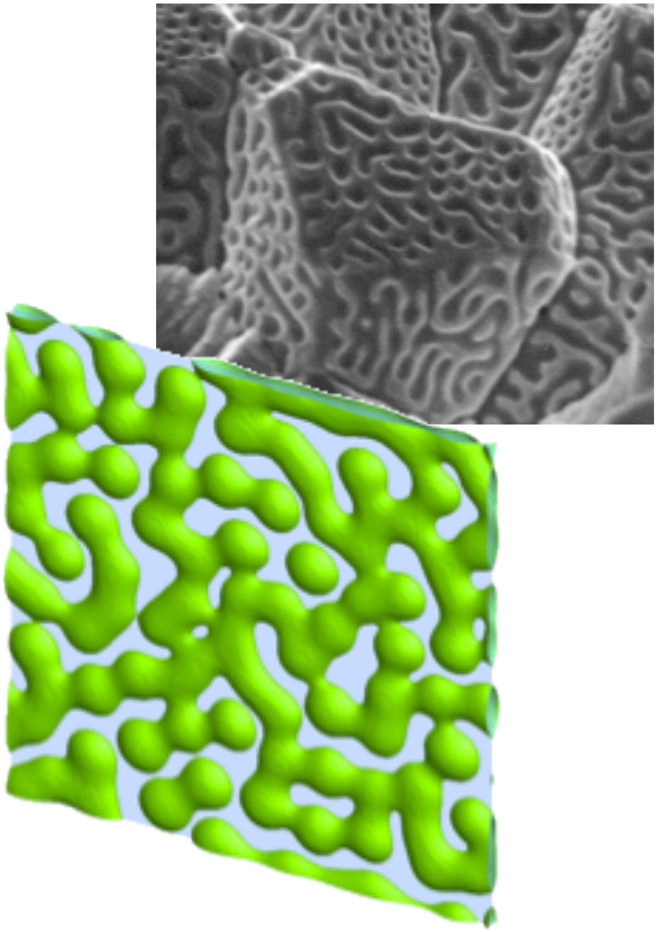
Void and GB Interaction in a Temperature Gradient



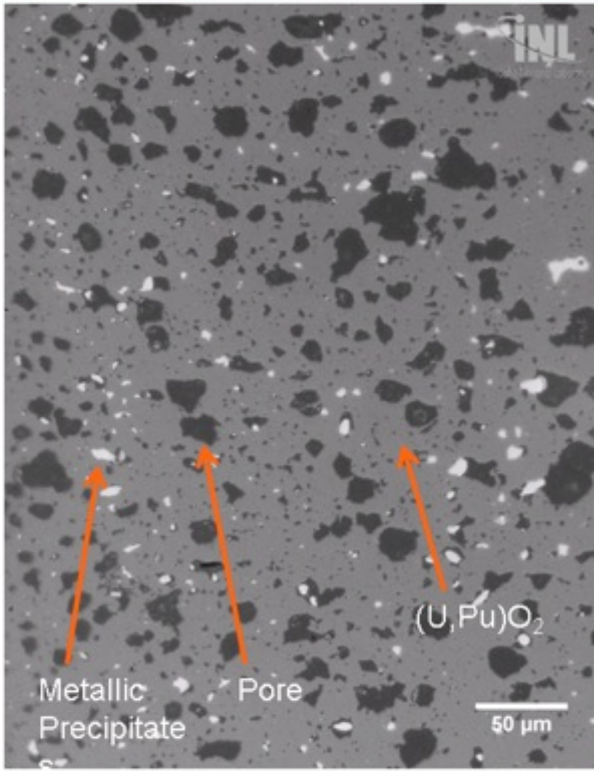


Why is coupling experiments to modeling and simulation important?

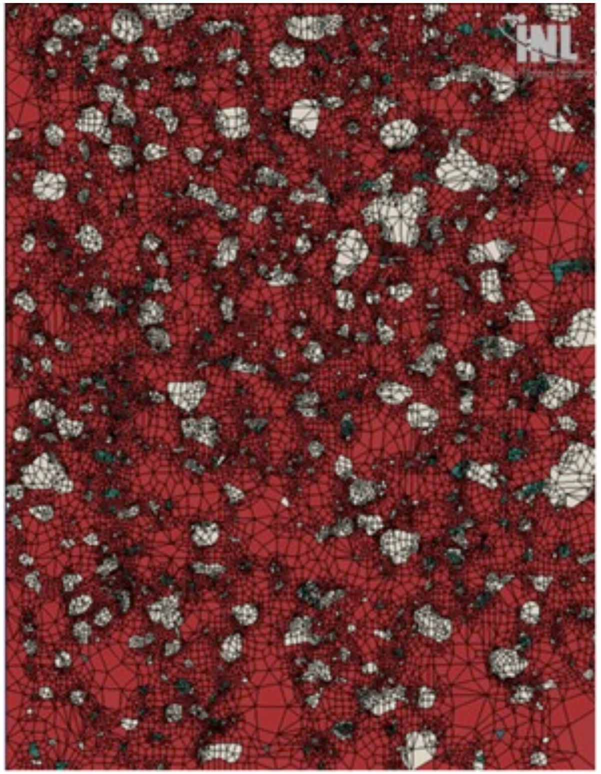
- Experimental results are used to validate/benchmark simulation results (without validation, models are just mathematics)
- Experimental data can provide the initial condition for simulations
- Simulations can predict behavior of “experiments” that would be impossible to perform
- Modeling and simulation can help target the experiment design process, to produce better data more cheaply



Putting real microstructures into FEA Models



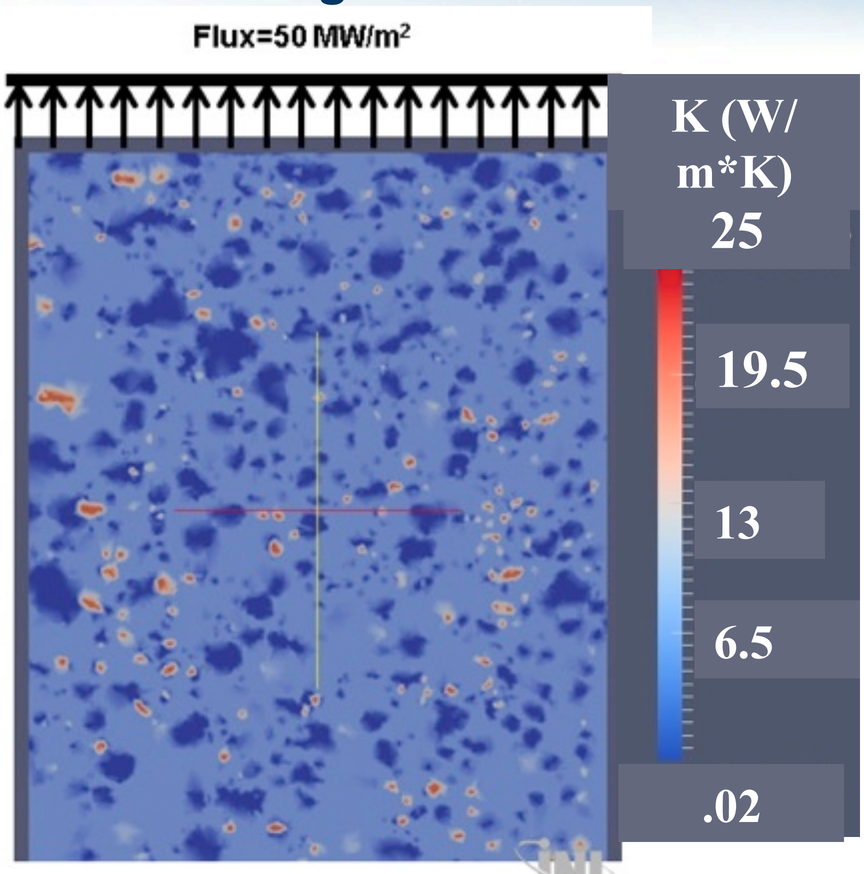
Optical Micrograph from High Burn-up ACO-3 MOX Fuel

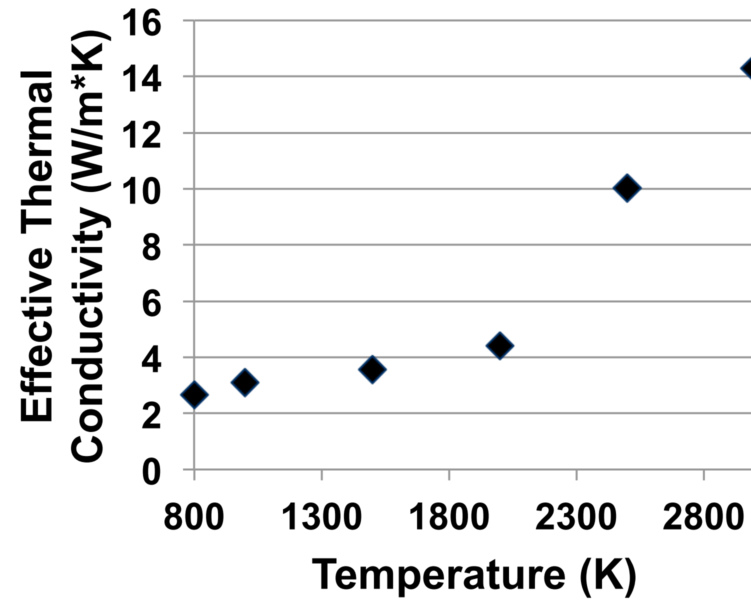


FEA Mesh Generated from Micrograph

- Meshes are generated using Object Oriented Finite Element Analysis (OOF) software
- Materials are discretely meshed, allowing for assignment of different material properties to the various phases

“Measuring” Effective Thermal Conductivities of microstructures





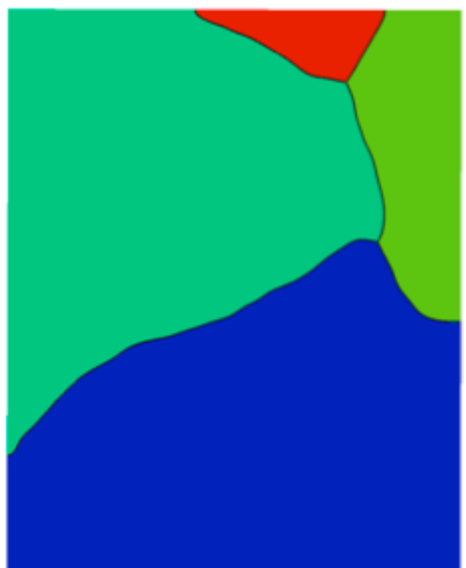
- Essentially a virtual laser flash diffusivity measurement is performed on the microstructure
- Running the model at a variety of temperature allows for development of a model for effective thermal conductivity

Microstructure Modeling with Real Initial Conditions

- In order to accurately model the microstructure evolution, we must have an accurate representation of the initial microstructure
- We are currently developing the capability to reconstruct the initial microstructure from EBSD scans (LDRD funded)

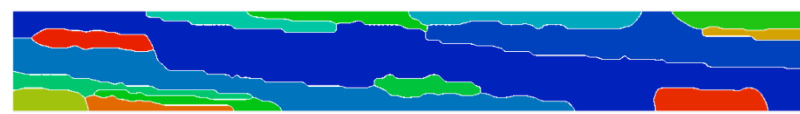
Microstructures can either be reconstructed exactly or be simplified

EBSD Scan



Reconstruction in MARMOT

EBSD Scan



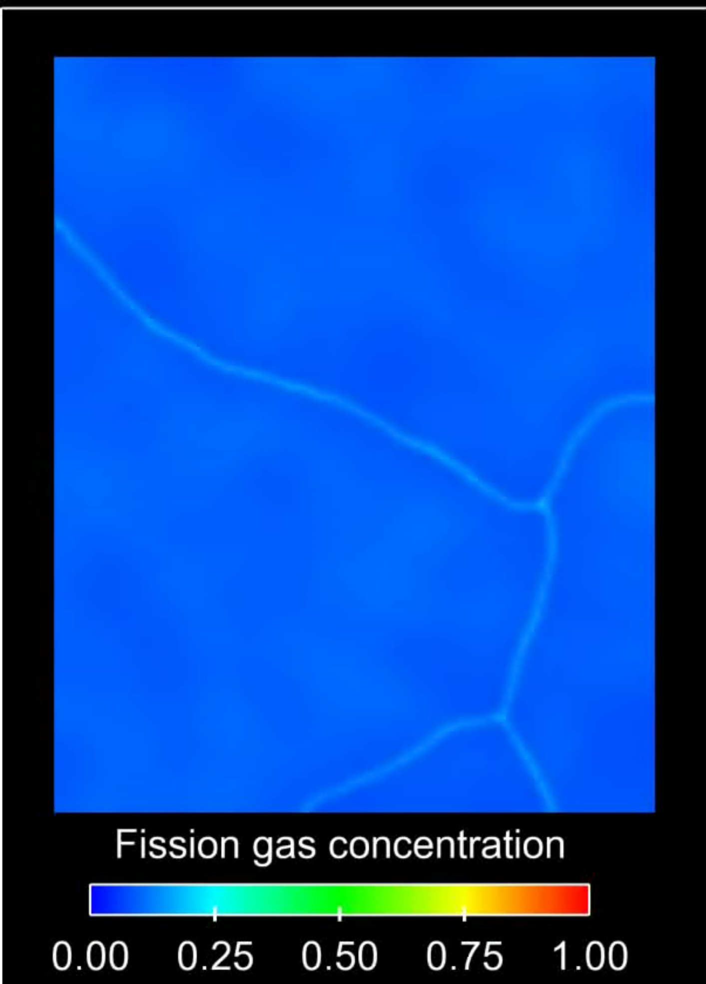
Approximated microstructure in MARMOT

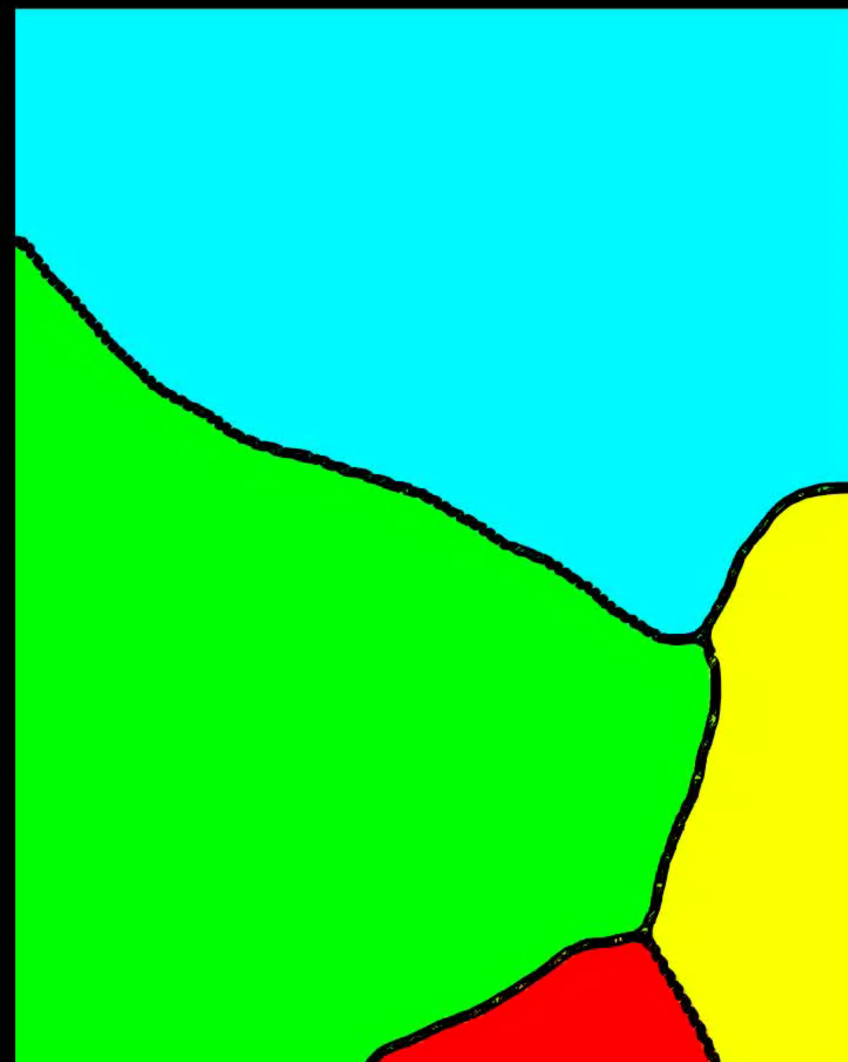
Fission Gas Segregation in a Reconstructed Microstructure

Idaho National Laboratory

MOOSE

MARMOT

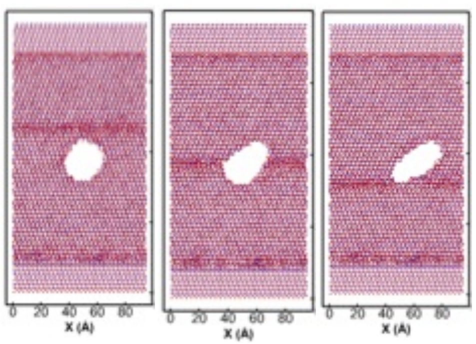




Conclusions

- A state variable model will allow for a more predictive fuel performance modeling capability
  - Variable evolution models are needed
  - Expressions defining the effect of state variables on material parameters are also needed

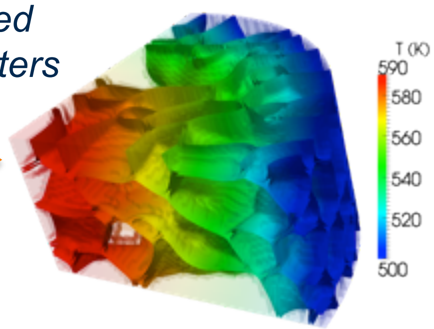
Atomistic simulation

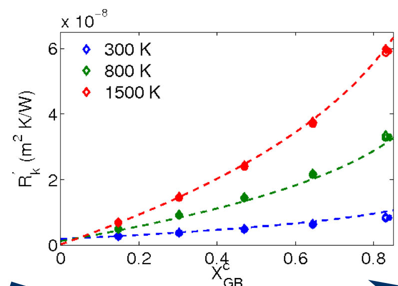


- Identify important mechanisms
- Determine material parameter values

Mesoscale models

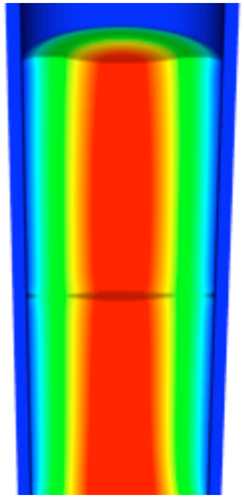
Atomistically-informed parameters





- Predict and define microstructure and state variable evolution
- Determine effect of evolution on material properties

Fuel performance models



- Predict fuel performance and failure